Violation of Wiedemann-Franz law at the Kondo breakdown quantum critical point

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We study both the electrical and thermal transport near the heavy-fermion quantum critical point (QCP), identified with the breakdown of the Kondo effect as an orbital selective Mott transition. We show that the contribution to the electrical conductivity comes mainly from conduction electrons while the thermal conductivity is given by both conduction electrons and localized fermions (spinons), scattered with dynamical exponent $z = 3$. This scattering mechanism gives rise to a quasi-linear temperature dependence of the electrical and thermal resistivity. The characteristic feature of the Kondo breakdown scenario turns out to be emergence of additional entropy carriers, that is, spinon excitations. As a result, we find that the Wiedemann-Franz ratio should be larger than the standard value, a fact which enables to differentiate the Kondo breakdown scenario from the Hertz-Moriya-Millis framework.

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Existence of quasiparticles is the cornerstone in Landau's Fermi-liquid theory [1] for modern theory of metals. Since they transport not only electric charge but also entropy, one sees that the ratio ($L = \frac{\kappa}{T\sigma}$) between thermal ($\kappa$) and electrical ($\sigma$) conductivities is given by a universal number $L_0 = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 = 2.45 \times 10^{-8} W\Omega K^{-2}$ [2], provided quasiparticles do not lose their energy during collisions, and certainly satisfied at zero temperature in the Landau Fermi liquid theory. Not only conventional metals [3] but also strongly correlated metals such as heavy fermions [4] turn out to follow the Wiedemann-Franz (WF) law [5]. In particular, even quantum critical metals of $CeNi_2Ge_2$ [6], $CeRhIn_5$ [7], and $CeCoIn_5$ [8] have shown to satisfy the WF law at least in the zero temperature limit, thus validating the quasiparticle picture, although their resistivities deviate from the conventional T^2 behavior.

Several years ago, violation of the WF law was observed in the optimally electron-doped cuprate $(Pr, Ce)_2CuO_4$ [4] and hole-underdoped cuprate $La_{2-x}Sr_xCuO_4$ [9] while the WF law turns out to hold in the overdoped cuprate $Tl_2Ba_2CuO_{6+\delta}$ [10], suggesting emergence of non-Fermi liquid physics as proximity of a Mott insulator. Recently, anisotropic violation of the WF law has been reported near the quantum critical point (QCP) of a typical heavy-fermion compound $CeCoIn_5$, where only c-axis transport violates the WF law while ab-plane transport follows it [11]. In this experiment the authors speculated that the temperature quasi-linear electrical resistivity and vanishing spectral weight may be one common feature for such non-Fermi liquid physics. In this respect they naturally proposed to observe violation of the WF law in $YbRh_2Si_2$ as another typical heavy-fermion compound exhibiting similar non-Fermi liquid physics with the c-axis measurement of $CeCoIn_5$, where both ab- and c- axis transport show the temperature quasi-linear electrical resistivity and vanishing spectral weight [12].

Physically, one can expect violation of the WF law as proximity of Mott physics or superconductivity away from quantum criticality, and as emergence of non-Fermi liquid physics near QCPs. In a Mott insulator the presence of charge gap makes electrical conductivity vanish, but gapless spin excitations can carry entropy, causing $L > L_0$ while Cooper pairs transport electric currents without entropy in the superconducting state, resulting in $L < L_0$. On the other hand, entropy is enhanced near QCPs due to critical fluctuations, and violation of the WF law is expected in principle.

In this paper we examine thermal transport and violation of the WF law based on the Kondo breakdown scenario [13, 14] as one possible heavy-fermion quantum transition for $YbRh_2Si_2$. This scenario differs from the standard model of quantum criticality in a metallic system, referred as the Hertz-Moriya-Millis framework [15], in respect that in the former case the whole heavy Fermi surface is destabilized at the QCP.

Several heavy-fermion compounds have been shown not to follow the SDW theory [12, 16, 17, 18]. Strong divergence of the effective mass near the QCP [16] and the presence of localized magnetic moments at the transition towards magnetism [17] seem to support a more exotic scenario. In addition, rather large entropy and small magnetic moments in the antiferromagnetic phase may be associated with antiferromagnetism out of a spin liquid Mott insulator [19]. Combined with the Fermi surface reconstruction at the QCP [16, 18], this quantum transition is assumed to show breakdown of the Kondo effect as an orbital selective Mott transition [19, 20], where only the f-electrons experience the metal-insulator transition.

Our main result is that the WF law should be violated at the Kondo breakdown QCP as proximity of spin liquid Mott physics, thus $L > L_0$, resulting from the presence of additional entropy carriers, here spinon excitations. This result may be opposed to the preservation of the WF law in the SDW framework [6].

We start from the U(1) slave-boson representation of the Anderson lattice model (ALM) in the large-U limit

$$\begin{aligned} L_{ALM} &= \sum_i c_{i\sigma}^\dagger(\partial_\tau - \mu)c_{i\sigma} - t\sum_{\langle ij\rangle}(c_{i\sigma}^\dagger c_{j\sigma} + H.c.) \\ &+V\sum_i(b_i f_{i\sigma}^\dagger c_{i\sigma} + H.c.) + \sum_i b_i^\dagger \partial_\tau b_i \\ &+\sum_i f_{i\sigma}^\dagger(\partial_\tau + \epsilon_f)f_{i\sigma} + J\sum_{\langle ij\rangle}(f_{i\sigma}^\dagger \chi_{ij} f_{j\sigma} + H.c.) \\ &+i\sum_i \lambda_i(b_i^\dagger b_i + f_{i\sigma}^\dagger f_{i\sigma} - 1) + NJ\sum_{\langle ij\rangle}|\chi_{ij}|^2. \end{aligned} \quad (1)$$

Here, $c_{i\sigma}$ and $d_{i\sigma} = b_i^\dagger f_{i\sigma}$ are conduction electron with a chemical potential μ and localized electron with an energy level ϵ_f, where b_i and $f_{i\sigma}$ are holon and spinon, associated with hybridization and spin fluctuations, respectively. The spin-exchange term for the localized orbital is introduced for competition with the hybridization term, and decomposed via exchange hopping processes of spinons, where χ_{ij} is a hopping parameter for the decomposition. λ_i is a Lagrange multiplier field to impose the single occupancy constraint $b_i^\dagger b_i + f_{i\sigma}^\dagger f_{i\sigma} = N/2$, where N is the number of fermion flavors with $\sigma = 1, ..., N$.

Performing the saddle-point approximation of $b_i \to b$, $\chi_{ij} \to \chi$, and $i\lambda_i \to \lambda$, one finds an orbital selective Mott transition as Kondo breakdown at $J \approx T_K$, where a spin-liquid Mott insulator ($\langle b_i\rangle = 0$) arises in $J > T_K$ while a heavy-fermion Fermi liquid ($\langle b_i\rangle \neq 0$) results in $T_K > J$ [13, 14, 19]. Here, $T_K = D\exp\Big(\frac{\epsilon_f}{N\rho_c V^2}\Big)$ is the single-ion Kondo temperature, where $\rho_c \approx (2D)^{-1}$ is the density of states for conduction electrons with the half bandwidth D.

One can read the WF ratio in the mean-field approximation. In the heavy-fermion phase it is given by $L = L_0$, representing a Fermi liquid state of heavy quasiparticles with a large Fermi surface. On the other hand, it becomes

$$L = L_0\Big(\frac{t + J\chi}{t}\Big)^2$$

in the spin liquid phase, where t is the hopping of the conduction electrons and χ is the spin liquid parameter. By contrast, in the U(1) slave-boson mean-field theory of the t-J Hamiltonian,

$$H_{tJ}^{MF} = \sum_{\langle ij\rangle}\Big\{NJ|\chi_{ij}|^2 - (t\delta + J\chi_{ij})f_{j\sigma}^\dagger f_{i\sigma} - H.c.\Big\},$$

where the holon field is replaced with its mean-field value of $b_i = \sqrt{\delta}$ with hole concentration δ, one finds $L = L_0\Big(\frac{t\delta + J\chi}{t\delta}\Big)^2$ [21], which represents a strong violation of the WF law at the vicinity of the insulating phase. This comparison tells us that the orbital selective Mott transition in the ALM has milder violation of the WF law than the single-band Mott transition although the underdoped state of the t-J model may have similarity with the fractionalized Fermi liquid [19] of the ALM.

Fluctuation-corrections are treated in the Eliashberg framework [13]. The main physics is that the Kondo breakdown QCP is multi-scale. The dynamics of the hybridization fluctuations is described by $z = 3$ critical theory due to Landau damping of electron-spinon polarization above an intrinsic energy scale E^*, while by $z = 2$ dilute Bose gas model below E^*, where z is the dynamical exponent. The energy scale E^* originates from the mismatch of the Fermi surfaces of the conduction electrons and spinons, shown to vary from $\mathcal{O}(10^0)\ mK$ to $\mathcal{O}(10^2)\ mK$. Based on the $z = 3$ quantum criticality, a recent study [22] has fitted the divergent Grüneisen ratio with an anomalous exponent 0.7.

Transport coefficients can be found from the following transport equations

$$\begin{aligned} \vec{J}_{el}^{c,f,b} &= K_0^{c,f,b}(\alpha_{c,f,b}\vec{E} + \beta_{c,f,b}\vec{\epsilon} - \vec{\nabla}\mu_{c,f,b}) + K_1^{c,f,b}\Big(\frac{-\vec{\nabla}T}{T}\Big), \\ \vec{J}_{th}^{c,f,b} &= K_1^{c,f,b}(\alpha_{c,f,b}\vec{E} + \beta_{c,f,b}\vec{\epsilon} - \vec{\nabla}\mu_{c,f,b}) + K_2^{c,f,b}\Big(\frac{-\vec{\nabla}T}{T}\Big). \end{aligned} \quad (2)$$

$\vec{J}_{el(th)}^{c,f,b}$ is an electric (thermal) current for conduction electrons, spinons, and holons, respectively, and $\vec{E}$, $\vec{\epsilon}$, $\mu_{c,f,b}$, and T are an external electric field, internal one, each chemical potential, and temperature, respectively, where $\alpha_{c,f,b} = 1, 0, -1$ and $\beta_{c,f,b} = 0, 1, 1$. $K_0^{c,f,b}$, $K_1^{c,f,b}$, and $K_2^{c,f,b}$ are associated with electrical conductivity, thermoelectric conductivity, and thermal conductivity for each excitation, respectively. Obtaining $\vec{\epsilon}$ from the current constraint $\vec{J}_{el}^f + \vec{J}_{el}^b = 0$ with $\mu_c = \mu_f - \mu_b$, and considering the open-circuit boundary condition, we find physical response functions for electrical conductivity σ_t, thermoelectric conductivity p_t, and thermal conductivity κ_t,

$$\begin{aligned} &\sigma_t = \sigma_c + \frac{\sigma_b\sigma_f}{\sigma_b + \sigma_f}, \qquad p_t = p_c + \frac{\sigma_b p_f - \sigma_f p_b}{\sigma_b + \sigma_f}, \\ &\frac{\kappa_t}{T} = \frac{\kappa_c}{T} + \frac{\kappa_f}{T} + \frac{\kappa_b}{T} - \frac{(p_b + p_f)^2}{\sigma_b + \sigma_f} - \frac{p_t^2}{\sigma_t} \end{aligned} \quad (3)$$

with $\sigma_{c,f,b} \equiv K_0^{c,f,b}$, $p_{c,f,b} \equiv K_1^{c,f,b}/T$, and $\kappa_{c,f,b} \equiv K_2^{c,f,b}/T$. One can also derive this general expression from the path-integral representation with the covariant derivative $\vec{D} = \vec{\nabla} - i\vec{A}_{el} - i\vec{A}_{th}(i\partial_\tau)$ in the continuum approximation, where $\vec{A}_{el}$ and $\vec{A}_{th}$ are external electromagnetic and thermal vector potential fields, respectively. We note that this expression reduces to that of the t-J model, when contributions from the conduction electrons are neglected [23].

It is straightforward to evaluate all current-current cor-

relation functions in the one loop approximation. We find

$$\sigma_c(T) = \mathcal{C}\rho_c v_F^{c2}\tau^b_{c,sc}(T),$$
$$\sigma_f(T) = \frac{\mathcal{C}\rho_f v_F^{f2}}{[\tau^b_{f,sc}(T)]^{-1} + [\tau^a_{f,tr}(T)]^{-1}},$$
$$p_c(T) = \frac{\pi^2}{3}\frac{c_F}{\epsilon_F}T\sigma_c(T), \quad p_f(T) = \frac{\pi^2}{3}\frac{c_F}{\epsilon_F}T\sigma_f(T),$$
$$\frac{\kappa_c(T)}{T} = \frac{\pi^2}{3}\sigma_c(T), \quad \frac{\kappa_f(T)}{T} = \frac{\pi^2}{3}\sigma_f(T) \quad (4)$$

with $\mathcal{C} = \frac{N}{\pi}\int_{-\infty}^{\infty} dy \frac{1}{(y^2+1)^2}$. In the electrical conductivity $\rho_{c(f)}$ and $v_F^{c(f)}$ are density of states and Fermi velocity for conduction electrons (spinons), respectively. $\tau^b_{c(f),sc}(T) = [\Im\Sigma_{c(f)}(T)]^{-1}$ is the scattering time due to $z = 3$ hybridization fluctuations, given by

$$\Im\Sigma_{c(f)}(T > E^*) = \frac{m_b V^2}{12\pi v_F^{f(c)}} T \ln\Big(\frac{2T}{E^*}\Big),$$
$$\Im\Sigma_{c(f)}(T < E^*) = \frac{m_b V^2}{12\pi v_F^{f(c)}} \frac{T^2}{E^*}\ln 2,$$

where $m_b = (2NV^2\rho_c)^{-1}$ is the band mass for holons. Note that hybridization fluctuations are gapped at $T < E^*$, resulting in the Fermi liquid like correction. $\tau^a_{f,tr}(T) = \Big\{\Big(\frac{k_F^f}{16\pi N}\Big)\gamma_a^{\frac{2}{3}} T^{\frac{5}{3}}\Big\}^{-1}$ is the transport time associated with $z = 3$ gauge fluctuations, where $\gamma_a \approx \pi/v_F^f$ is the Landau damping coefficient for gauge fluctuations and k_F^f is the Fermi momentum of spinons. In the thermoelectric coefficient ϵ_F is the Fermi energy for conduction electrons, and c_F is a geometrical factor, here $c_F = 3/2$ for the spherical Fermi surface [24].

Several remarks are in order for each transport coefficient. An important point is that the vertex corrections for scattering with hybridization fluctuations can be neglected, a unique feature of the two band model, resulting from heavy mass of spinons [13, 14]. This allows us to replace the transport time with the scattering time for such a process. On the other hand, vertex corrections for scattering with gauge fluctuations turn out to be crucial, where infrared divergence of the self-energy correction at finite temperatures is cancelled via the vertex correction, giving rise to gauge-invariant [25] finite physical conductivity [26]. As a result, the gauge non-invariant divergent spinon self-energy $\Im\Sigma^a_f(T)$ in $\Im\Sigma^b_f(T) + \Im\Sigma^a_f(T)$ of the conductivity expression is replaced with the gauge invariant finite transport time $[\tau^a_{f,tr}(T)]^{-1}$. Both irrelevance (hybridization fluctuations) and relevance (gauge fluctuations) of vertex corrections can be also checked in the quantum Boltzman equation study.

Both the thermoelectric and thermal conductivities are nothing but the Fermi liquid expressions, where each fermion sector satisfies the WF law. Although inelastic scattering with both hybridization and gauge fluctuations may modify the Fermi liquid expressions beyond the one-loop approximation, the WF law for each fermion sector will be preserved at least in the zero temperature limit, where such inelastic scattering processes are suppressed. One may regard the WF law for each fermion sector as the most important assumption in this paper.

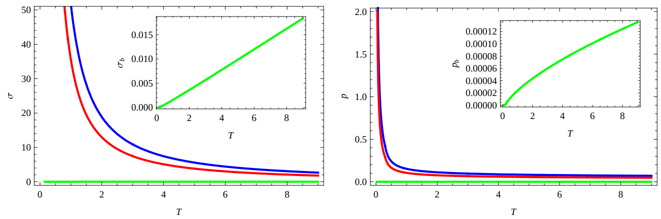

FIG. 1: (Color online) Left: Electrical conductivity from conduction electrons (blue), spinons (red), and holons (green). Left-inset: Electrical conductivity from holons much smaller than contributions from fermions. Right: Thermoelectric conductivity from conduction electrons (blue), spinons (red), and holons (green). Right-inset: Thermoelectric conductivity from holons much smaller than contributions from fermions.

Transport coefficients for holon excitations turn out to be much smaller than fermion contributions, that is, $\sigma_c(T) \geq \sigma_f(T) \gg \sigma_b(T)$, $p_c(T) \geq p_f(T) \gg p_b(T)$, and $\kappa_c(T) \geq \kappa_f(T) \gg \kappa_b(T)$ as clearly shown in Fig. 1, thus irrelevant. Physically the dominance of fermion contributions can be understood from an argument of density of states. Since there are many states at the Fermi surface in the vacuum state, their conductivities diverge in the clean limit as the temperature goes down to zero. On the other hand, there are no bosons at zero temperature, thus their conductivity vanishes when $T \to 0$.

Inserting all contributions into Eq. (3), we find the physical transport coefficients near the Kondo breakdown QCP. Interestingly, the dominance of fermion contributions allows us to simplify the total transport coefficients as

$$\sigma_t(T) \approx \sigma_c(T) = \mathcal{C}\rho_c v_F^{c2}\tau^c_{sc}(T),$$
$$p_t(T) \approx p_c(T) = \frac{\pi^2}{3}\frac{c_F}{\epsilon_F}T\sigma_c(T),$$
$$\frac{\kappa_t(T)}{T} \approx \frac{\kappa_c(T)}{T} + \frac{\kappa_f(T)}{T} = \frac{\pi^2}{3}\Big(\sigma_c(T) + \sigma_f(T)\Big). \quad (5)$$

Actually, we have checked that each approximate formula matches with each total expression. The main point is that spinons participate in carrying entropy, enhancing the thermal conductivity, while both electric and thermoelectric conductivities result from conduction electrons dominantly.

Fig. 2 shows the quasi-linear behavior in temperature for both electrical and thermal resistivities above E^*, resulting from scattering with $z = 3$ hybridization fluctuations dominantly, because of $[\tau^b_{f,sc}(T)]^{-1} \gg [\tau^a_{f,tr}(T)]^{-1}$ in the spinon conductivity, explicitly checked from numerical analysis and temperature dependence, thus $\sigma_f(T) \approx \mathcal{C}\rho_f v_F^{f2}\tau^b_{f,sc}(T)$. Here, we have used parameters of Ref. [22], shown to be successful for fitting of Grüneisen ratio.

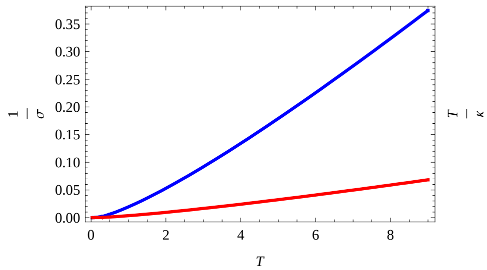

FIG. 2: (Color online) Quasi-linear electrical (blue) and thermal (red) resistivity above E^*, where thermal resistivity is smaller than electrical resistivity owing to the contribution from spinon excitations.

The WF ratio is given by

$$L(T) \equiv \frac{\kappa_t(T)}{T\sigma_t(T)} \approx \frac{\kappa_c(T) + \kappa_f(T)}{T\sigma_c(T)} \approx L_0\Big(1 + \frac{\rho_f v_F^f}{\rho_c v_F^c}\Big) \quad (6)$$

in the low temperature limit, where gauge-fluctuation corrections are irrelevant compared with hybridization-fluctuation corrections, thus ignored in the last expression.

The larger value of the WF ratio is the characteristic feature of the Kondo breakdown scenario, resulting from additional entropy carriers, here the spinon excitations. If we perform the transport study based on the SDW theory in the same approximation as the present framework, we will find $\sigma_t(T) \propto \tau_{tr}(T)$, $p_t(T) = \frac{\pi^2}{3}\frac{c_F}{\epsilon_F}T\sigma_t(T)$, and $\frac{\kappa_t(T)}{T} = \frac{\pi^2}{3}\sigma_t(T)$, where likewise contributions from critical boson excitations are assumed to be irrelevant, and the scattering time is replaced with the transport time. As a result, the WF law is expected to hold although non-Fermi liquid physics governs the quantum critical regime. Actually, this has been clearly demonstrated in the self-consistent renormalization theory, well applicable to $CeNi_2Ge_2$ [6]. In this respect the violation of the WF law discriminates the Kondo breakdown scenario from the SDW framework.

In this study we have ignored thermal currents driven by gauge fluctuations, known to be the phonon-drag effect in the electron-phonon system [24]. Recently, Nave and Lee have considered such photon-drag effects in the spin liquid context with $z = 3$ gauge fluctuations based on quantum Boltzmann equations, and argued that drag effects are subdominant, compared with fermion contributions [27]. Resorting to their conclusion, we argue that dominant thermal currents are driven by fermion excitations, here both conduction electrons and spinons.

In conclusion, we found marginal Fermi liquid physics for both electrical and thermal transport near the Kondo breakdown QCP due to scattering with $z = 3$ hybridization fluctuations. Our main discovery is that the Kondo breakdown QCP should violate the WF law at least in the zero temperature limit due to proximity of spin liquid Mott physics, i.e., existence of additional entropy carriers, that is, spinons.

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